

Biphenyl

92-52-4 | DTXSID4020161

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.47e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.04e-01

Confidence level: 5.21e-01

Nearest Neighbors from the Training Set

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Octachlorocyclopentene

Measured: 2.91e-07

Predicted: 1.00e-06

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Propane, 1,3-dibromo-2,2-bis(bromomethyl)-

Measured: 4.13e-06

Predicted: 7.44e-06

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Hexachlorocyclopentadiene

Measured: 6.60e-06

Predicted: 9.10e-06

Image not found

1-Chloronaphthalene

Measured: 1.07e-04

Predicted: 4.39e-05

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2-Chloronaphthalene

Measured: 7.19e-05

Predicted: 3.77e-05